



chain nodes :

7 9 12 13 15 16 17 19

ring nodes :

1 2 3 4 5 6

chain bonds :

1-9 4-7 12-13 15-16 17-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-9 4-7 12-13 15-16 17-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G3:X,CH2,CF3,CCl3,CO2H,CN,SO3H,CHO,C(O)CH3

G4:X,Ak,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,NO2

G5:H,NO2,X,Cb,Cy,Hy,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 12:CLASS 13:CLASS 15:CLASS
16:CLASS 17:CLASS 19:CLASS